ANALYSIS OF THE HIGH RESOLUTION ROTATIONAL SPECTRUM OF 2-CHLOROETHANOL

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2-Chloroethanol ($HOCH_2CH_2Cl$) is the smallest terrestrially stable chlorohydrin and is predicted to exist in the interstellar medium, forming from HCl with either oxirane or ethylene glycol, each of which are known interstellar constituents. Rotational[a] and ro-vibrational [b, c] spectra of 2-chloroethanol have been previously reported from 9-40 GHz and 100-500 cm^{-1}, respectively. However, attempts at the detection of 2-chloroethanol towards Sgr B2(N) have been unsuccessful. It is uncertain if the lack of detection arises from its lack of presence in this sightline, or whether the extrapolated spectral information for 2-cholorethanol is not of sufficient accuracy to guide astronomical searches. Therefore, we have measured the spectrum of 2-chloroethanol from 140 to 700 GHz to further improve the molecular constants and provide spectral frequencies directly comparable to radio telescope data. Analysis of this spectrum has resulted in the determination of refined rotational constants and centrifugal distortion constants up to the octic level for both naturally occurring Cl isotolopologues. Partially resolved nuclear quadrupole coupling arising from the presence of the chlorine atom is observed throughout the spectral range. New spectra from 8 to 26 GHz have been obtained to refine the quadrupole coupling constants with well resolved microwave transitions. We also have tentative least-squares fits of transitions for all vibrationally excited states below 500 cm^{-1} for each isotopologue, where the majority appear to be perturbed by Coriolis interactions. Analysis of the vibrationally excited states will be facilitated by the previously published high resolution far-IR data and may provide new insights into the vibrational energies and coupling interactions of these states. Here we will report the in-depth spectral analysis of the rotational spectrum of 2-chloroethanol.

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